



1/5

Sequence Alignment for mmp-8, mmp-3, and mmp-1

	85	90	100	110	120
h-mmp8	NPKWERTNL	TYRIRNYTPQL	SEAEVERAI	KDAFEL	WSVAS
h-mmp3	IPKWRKTHL	TYRIVNYTPDL	PKDAVDS	AVEKALK	VWEEVT
h-mmp1	NPRWEQTHL	TYRIENYTPDL	PRADVDA	IEKAFQL	WSNVT
	* . *	* . *	* . *	* . *	* . *

	130	140	150	160
h-mmp8	PLIFTRISQGEADINIAFYQRDHGDNSPFDGPNGLAHAF			
h-mmp3	PLTFSRLYEGEADIMISFAVREHGDFYPFDGPGNVLAHAY			
h-mmp1	PLTF TKVSEGQADIMISFVRGDHRDNSPFDGPGGNLAHAF			
	** * . . . *	* . *	* . *	* . *

	170	180	190	200
h-mmp8	QPGQGIGGDAHFDAEETWTNTSANYNLF	LVA	AHE	FGHSLG
h-mmp3	APGPGINGDAHFDDDEQWTKDTTGTNLF	LVA	AHE	IGHSLG
h-mmp1	QPGPGIGGDAHFDEDERWTNNFREYNLH	RVA	AHE	LGHSLG
	****	*****	* . *	** *****

	210	220	230	240
h-mmp8	LAHSSDPGALMYPNY-AFRETSNYSLP	QDDIDG	IQAIYG	
h-mmp3	LFHSANTEALMYPLYHSLTDLTRFRLS	QDDING	IQSLYG	
h-mmp1	LSHSTDIGALMYPSTY-TF--SGDVQLA	QDDIDG	IQAIYG	
	* . *	*****	* . *	* . *

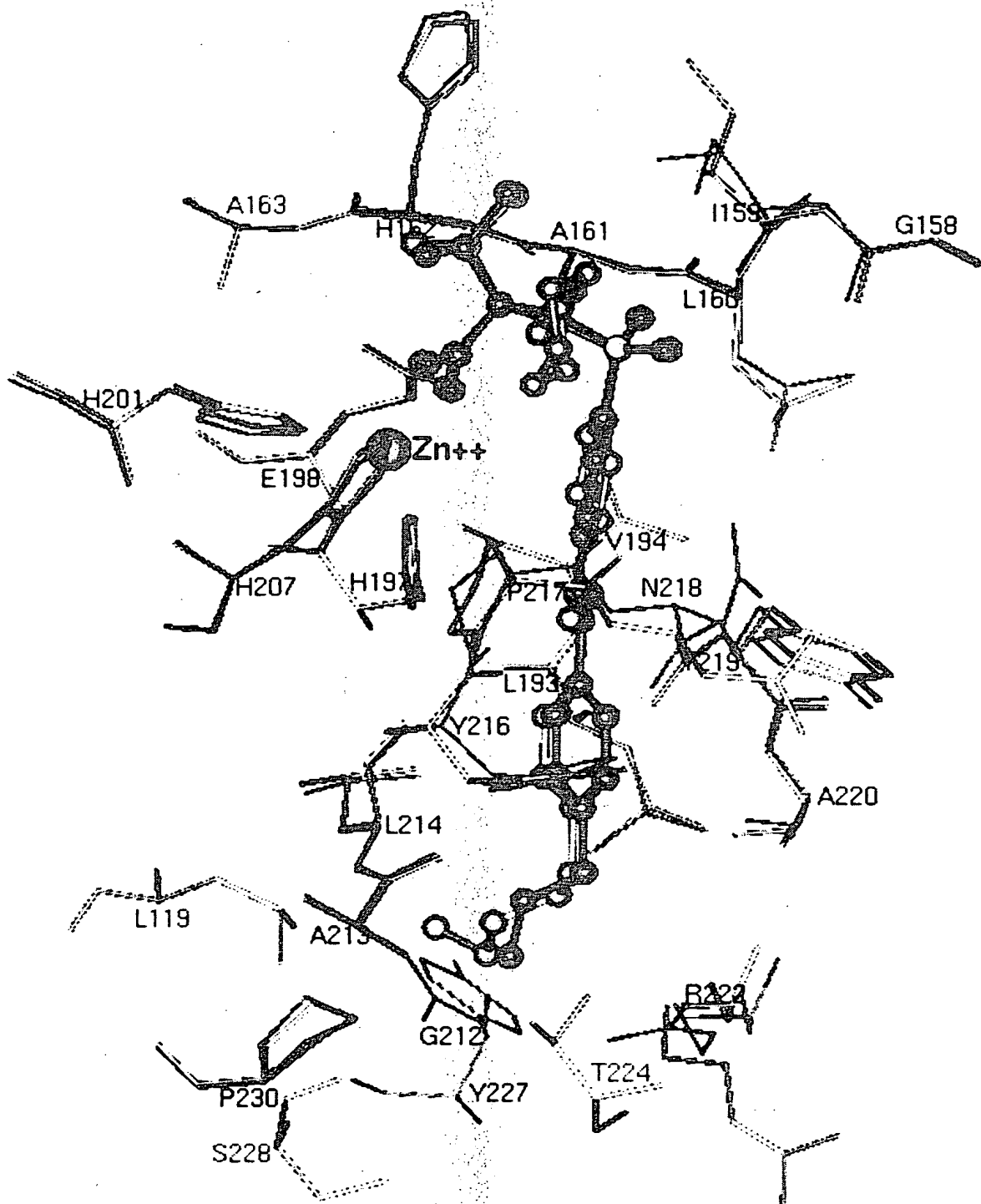
FIG.1

2/5

INTERACTING RESIDUES WITHIN 5 Å OF THE INHIBITOR MOLECULE							
		XII	IX	X	XI	XIV	
	L119	NO				NO	
	G158						
	I159						
	L160						
	A161						
	H162						
	A163	NO					
	L193						
	V194						
	A196	NO	NO		NO	NO	
	H197						
	E198						
	H201						
	H207						
	G212		NO	NO		NO	
	A213						
	L214						
	Y216						
	P217						
	N218						
	Y219						
	A220						
	R222						
	T224	NO				NO	
	Y227		NO	NO	NO	NO	
	S228	NO				NO	
	P230					NO	

FIG.2

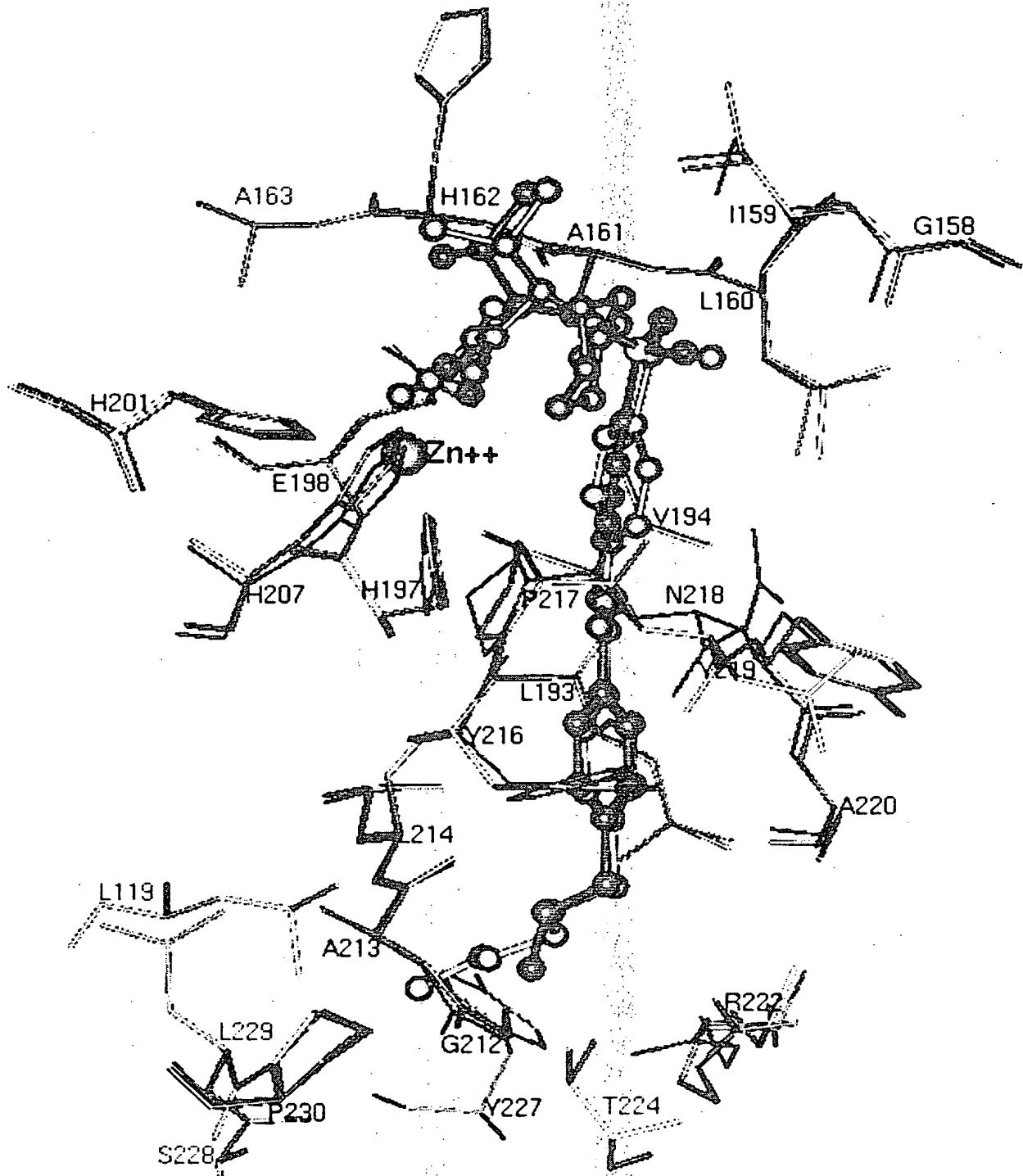
3/5



Surrounding Residues in mmp8 Active Site
(Inhibitors XII and IX)

FIG.3

4/5



Surrounding Residues in mmp8 Active Site
(Inhibitors XII and XI)

FIG.4

(ϕ , ψ) DISTRIBUTION AMONG THE RESIDUES FROM 222 TO 231

	222(R)	223(E)	224(T)	225(S)	226(N)					
I	-143.1	145.4	-50.0	128.2	-102.1	-14.3	-48.1	-31.1	-147.0	43.3
II	-132.7	133.2	-76.8	126.3	-112.1	134.8	-124.7	-16.2	-145.6	-174.7
III	-154.5	134.9	-73.5	145.4	-141.2	115.8	-89.0	-23.2	-136.0	-161.4
IV	-142.1	129.3	-74.5	134.3	-125.4	149.0	-128.8	-10.4	-144.1	-168.4
X1	-151.0	145.4	-48.5	130.0	-105.1	-10.5	-55.9	-29.2	-144.8	45.9
X2	-156.8	143.9	-43.9	129.5	-108.0	-9.7	-54.9	-29.8	-145.1	40.5

5/5

	227(Y)	228(S)	229(L)	230(P)	231(Q)					
I	-66.4	137.6	-139.7	147.8	-48.4	124.5	-60.7	152.7	-46.1	-44.3
II	-91.6	28.1	-86.5	126.1	-96.1	149.1	-59.7	152.2	-54.4	-35.0
III	-99.2	28.6	-92.2	127.0	-90.6	149.7	-61.1	155.6	-55.0	-42.0
IV	-97.7	21.7	-85.3	128.3	-85.4	159.9	-62.8	156.6	-56.3	-40.1
X1	-74.2	143.6	-143.0	153.8	-54.7	138.0	-66.6	158.4	-46.3	-51.6
X2	-70.4	140.5	-138.9	157.2	-54.4	136.8	-67.6	157.8	-46.1	-50.5

FIG.5